

Algebraic structure of Dirac fermion state in α -(BEDT-TTF)₂I₃

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We study the algebraic structure of the Dirac fermion state in the organic conductor, α -(BEDT-TTF)₂I₃. We find a pair of generators for the Hamiltonian of α -(BEDT-TTF)₂I₃ that describes the chirality of Dirac fermions. The phase parameters associated with those generators have an intimate and simple relationship with the positions of the Dirac points in the Brillouin zone. By making use of the form of the generators, a reduced form of the Hamiltonian is constructed that shares some characteristic features of the Dirac fermions with α -(BEDT-TTF)₂I₃. For the reduced Hamiltonian we present the analytic expression for the Dirac point position that sits at *arbitrary* point in the Brillouin zone determined by the hopping parameters.

KEYWORDS: Dirac fermion, α -(BEDT-TTF)₂I₃, organic conductor

1. Introduction

Massless Dirac fermion spectrums in two-spatial dimension are now realized in various condensed matter systems. A well-known system is graphene, a single atomic layer of graphite, which is a two-dimensional hexagonal lattice of carbon atoms.¹ The existence of the Dirac fermion spectrum was clearly demonstrated by the observation of the half-integer quantum Hall effect.^{2,3} Another example is a group of three-dimensional topological insulators⁴⁻⁶ where the surface state exhibits a Dirac fermion spectrum. A Dirac fermion spectrum appears even in superconductors. In the antiferromagnetic state of iron pnictide superconductors, a Dirac fermion spectrum^{7,8} was observed in angle-resolved photoemission spectroscopy.⁹ An organic compound, α -(BEDT-TTF)₂I₃ [BEDT-TTF=bis(ethylenedithio)tetrathiafulvalene], which has a layered structure of BEDT-TTF molecules, demonstrates that a Dirac fermion spectrum appears by suppressing strong electron correlation effects.¹⁰ Under ambient pressure, this compound undergoes a metal-insulator transition due to a charge ordering induced

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by a strong electron correlation.^{11–14} This charge ordering is suppressed by applying pressure, and transport measurements support the presence of a Dirac fermion spectrum^{15–18} for pressures higher than 1.5GPa. The presence of Dirac fermions is clearly demonstrated in the interlayer magnetoresistance measurement¹⁹ where the zero energy Landau level of Dirac fermions leads to negative magnetoresistance.²⁰

A natural question is how a Dirac fermion spectrum appears. In case of graphene, the mechanism is trivial. The Dirac fermion spectrum is realized as a result of symmetry of the honeycomb lattice. In case of topological insulators, essentially the spin-orbit interaction lead to a linear Dirac fermion energy spectrum.^{4–6, 21–23} In case of iron-pnictide superconductors, a characteristic configuration of Fe and As leads to degeneracy of d-orbitals at the Γ point, and supports the appearance of Dirac fermion spectrum.⁷ Contrary to these systems, the mechanism of stabilizing the Dirac fermion spectrum in α -(BEDT-TTF)₂I₃ is elusive.^{24, 25}

In Dirac fermion systems the conduction and the valence bands touch at two inequivalent points in the Brillouin zone (BZ). Usually reflecting symmetry of the system, the Dirac points appear at high symmetric points or along symmetric lines in the BZ. However, the Dirac points in α -(BEDT-TTF)₂I₃ are neither located at symmetric points of the BZ nor along symmetric lines in the BZ. So the presence of the Dirac fermion spectrum of this system is called accidental degeneracy.²⁶ Furthermore, the positions of the Dirac points depend on the applied pressure.^{10, 27} The complicated four band structure of α -(BEDT-TTF)₂I₃ prevents revealing the essential algebraic structure for the stabilization of the Dirac fermion spectrum.

In this paper, we study the underlying algebraic structure for the Dirac fermion spectrum in α -(BEDT-TTF)₂I₃. In spite of the complexity of the system, *i.e.*, the presence of many hopping parameters and multi-orbital character, there is a relatively simple algebraic structure that supports the Dirac fermion spectrum. We show that two matrices Γ_x and Γ_y describe chirality of Dirac fermions, and, interestingly, phase parameters contained in these matrices and the positions of the Dirac points are intimately connected in a simple functional relationship. Using the result, we construct a multi-orbital Hamiltonian with a Dirac fermion spectrum whose Dirac points move in the BZ by changing the hopping parameters.

The paper is organized as follows. In § 2 we consider graphene as a simple example to illustrate the algebraic structure of a Dirac fermion system. In § 3 we introduce the model for α -(BEDT-TTF)₂I₃, and we show a simple relationship between the matrices Γ_x and Γ_y and the positions of the Dirac points. In § 4 we construct a multi-orbital Hamiltonian that has a Dirac fermion spectrum whose Dirac points move by changing the hopping parameters. We also present the analytic expression for the Dirac point position in the BZ. In § 5 we summarize

the result.

2. Algebraic structure of graphene

In order to illustrate the algebraic structure of Dirac fermions we consider graphene as a simple example. The purpose is to extract the algebraic structure that is associated with chirality, which is one of the most characteristic properties of Dirac fermions.

Usually chirality is defined by using eigenstates of Dirac fermions.²⁸ In case of two component Dirac fermion wave functions, which is the most simplest Dirac fermion wave function, one can define a chirality vector field by $n_{k\alpha} = \langle \psi_k | \sigma_\alpha | \psi_k \rangle$ with ψ_k being a two-component Dirac fermion wave function at k in the Brillouin zone and σ_α being the Pauli matrices. The chirality vector has either a vortex or anti-vortex configuration around Dirac points. It is possible to construct this chirality vector field directly from the Hamiltonian by introducing two matrices or generators. We illustrate how this construction is carried out in graphene.

The Hamiltonian for graphene is given by²⁸

$$\mathcal{H} = \sum_k \begin{pmatrix} c_{Ak}^\dagger & c_{Bk}^\dagger \end{pmatrix} H_k \begin{pmatrix} c_{Ak} \\ c_{Bk} \end{pmatrix}, \quad (1)$$

where $c_{\alpha k}^\dagger$ ($c_{\alpha k}$) creates (annihilates) an electron with the wave vector \mathbf{k} on sublattice $\alpha = A, B$, and

$$H_k = \begin{pmatrix} 0 & \kappa_k \\ \kappa_k^* & 0 \end{pmatrix}, \quad (2)$$

with

$$\kappa_k = -t \left[e^{ik_x} + e^{i\left(-\frac{1}{2}k_x + \frac{\sqrt{3}}{2}k_y\right)} + e^{-i\left(\frac{1}{2}k_x + \frac{\sqrt{3}}{2}k_y\right)} \right]. \quad (3)$$

We set the lattice constant unity. Denoting a Dirac point in the BZ as \mathbf{k}_D , we find $\kappa_{\mathbf{k}_D} = 0$.

Expanding κ_k around $\mathbf{k} = \mathbf{k}_D$, we find that

$$\left. \frac{\partial \kappa_k}{\partial k_x} \right|_{\mathbf{k}=\mathbf{k}_D} = C_x \exp\left(-\frac{i}{2}k_{Dx}\right) i, \quad \left. \frac{\partial \kappa_k}{\partial k_y} \right|_{\mathbf{k}=\mathbf{k}_D} = C_y \exp\left(-\frac{i}{2}k_{Dx}\right),$$

where C_x and C_y are real constants. Note that there is the factor $\exp\left(-\frac{i}{2}k_{Dx}\right)$ that depends on \mathbf{k}_D in the right hand side of these equations. We encounter similar factors for the case of α -(BEDT-TTF)₂I₃ later. Introducing the following matrix,

$$\Gamma_\alpha = \left. \frac{\partial H_k}{\partial k_\alpha} \right|_{\mathbf{k}=\mathbf{k}_D},$$

and representing these matrices as $\Gamma_x = a_x(\sigma_x \cos \theta_x + \sigma_y \sin \theta_x)$ and $\Gamma_y = a_y(\sigma_x \cos \theta_y +$

$\sigma_y \sin \theta_y$), we find $|\theta_x - \theta_y| = \pi/2$. This phase difference $\pi/2$ comes from the phase difference between $\partial \kappa_k / \partial k_x|_{\mathbf{k}=\mathbf{k}_D}$ and $\partial \kappa_k / \partial k_y|_{\mathbf{k}=\mathbf{k}_D}$. If we define an inner-product between two matrices as $(A, B) = \text{tr}(AB) = \sum_{i,j} A_{ij} B_{ji}$, we find that $(\Gamma_x, \Gamma_y) = a_x a_y \cos(\theta_x - \theta_y) = 0$. because of the phase difference $\pi/2$.

Now we construct the chirality vector directly from the Hamiltonian using the matrices Γ_α . The 2×2 matrix H_k has the following form around the Dirac point:

$$H_{\mathbf{k}_D + \delta \mathbf{k}} = \Gamma_x \delta k_x + \Gamma_y \delta k_y + \cdots \quad (4)$$

Suppose one moves around the Dirac point. The path is represented by $\delta k_x = \delta k_0 \cos \phi$, $\delta k_y = \delta k_0 \sin \phi$, with ϕ changing from 0 to 2π . We define a vector field (n_{kx}, n_{ky}) as

$$n_{kx} = \text{tr}(\Gamma_x H_{\mathbf{k}}), \quad n_{ky} = \text{tr}(\Gamma_y H_{\mathbf{k}}), \quad (5)$$

It is easy to see that n_{kx} and n_{ky} vanish at Dirac points. As shown in Fig. 1, we find that this vector field rotates as one goes around the Dirac point. The vector field (n_{kx}, n_{ky}) forms vortex (anti-vortex) around the two inequivalent points. These points correspond to the Dirac points in graphene. Therefore, the vector field (n_{kx}, n_{ky}) describes the chirality of the Dirac fermion. Note that by symmetry the vector field (n_{kx}, n_{ky}) can be rotated in the $k_x - k_y$ plane, or one can define

$$n'_{kx} = \text{tr}(\Gamma'_x H_{\mathbf{k}}), \quad n'_{ky} = \text{tr}(\Gamma'_y H_{\mathbf{k}}), \quad (6)$$

with $\Gamma'_x = \Gamma_x \cos \phi - \Gamma_y \sin \phi$ and $\Gamma'_y = \Gamma_x \sin \phi + \Gamma_y \cos \phi$. In Fig. 1 we set $\Gamma_x = \sigma_x$ and $\Gamma_y = \sigma_y$ by making use of this symmetry.

In case of graphene, the analysis is trivial because we have only four matrices, the Pauli matrices σ_x , σ_y , σ_z , and the unit matrix σ_0 , to construct 2×2 Hamiltonians. Because of the absence of σ_0 and σ_z components in the graphene Hamiltonian, the space of matrices Γ_α is uniquely determined.

3. Algebraic structure of α -(BEDT-TTF) $_2$ I $_3$

Contrary to graphene, it is unclear how to find Γ_α matrices for the case of α -(BEDT-TTF) $_2$ I $_3$ because the Hamiltonian is 4×4 . (See, eq. (8) below.) There are 15 generators and one unit matrix for constructing 4×4 Hermite matrix. A suitably chosen set of those generators satisfy commutation relations similar to that for σ_x , σ_y , and σ_z . However, naive choices fail to describe chirality of Dirac fermions in α -(BEDT-TTF) $_2$ I $_3$.

In order to find Γ_α , we study the Hamiltonian of α -(BEDT-TTF) $_2$ I $_3$. We consider a single plane of BEDT-TTF molecules. The unit cell consists of four BEDT-TTF molecules, which

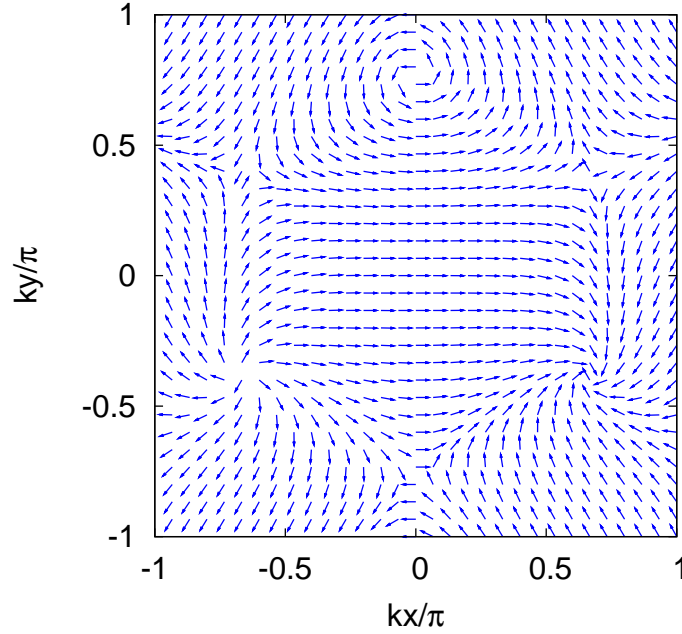


Fig. 1. The vector field (n_{k_x}, n_{k_y}) for graphene in \mathbf{k} space. The vector field is normalized to clarify the structure around the Dirac points. (We take the lattice constant as the unit of length.) The vector field forms vortex (anti-vortex) around K: $(2\pi/3)(1, 1/\sqrt{3})$ ($K': (2\pi/3)(1, -1/\sqrt{3})$). The points K and K' are the Dirac points. (A similar result was presented in ref. 29.)

are labeled by 1, 2, 3, and 4. The Hamiltonian is given by^{10,30}

$$\mathcal{H} = \sum_k c_k^\dagger H_k c_k, \quad (7)$$

where the spinor representation of the creation operator is $c_k^\dagger = \begin{pmatrix} c_{1k}^\dagger & c_{2k}^\dagger & c_{3k}^\dagger & c_{4k}^\dagger \end{pmatrix}$ and

$$H_k = \begin{pmatrix} 0 & t_{c1} + t_{c2}e^{-ik_y} & t_{p1} - t_{p4}e^{ik_x} & t_{p2} - t_{p3}e^{ik_x} \\ t_{c1} + t_{c2}e^{ik_y} & 0 & t_{p4}e^{ik_y} - t_{p1}e^{i(k_x+k_y)} & t_{p3} - t_{p2}e^{ik_x} \\ t_{p1} - t_{p4}e^{-ik_x} & t_{p4}e^{-ik_y} - t_{p1}e^{-i(k_x+k_y)} & 0 & t_{c3} + t_{c4}e^{-ik_y} \\ t_{p2} - t_{p3}e^{-ik_x} & t_{p3} - t_{p2}e^{-ik_x} & t_{c3} + t_{c4}e^{ik_y} & 0 \end{pmatrix}. \quad (8)$$

Here hopping parameters t_η ($\eta = c1, \dots, c4, p1, \dots, p4$) are assumed to be pressure dependent. There are two types of pressure: uniaxial pressure and hydrostatic pressure. For the purpose of investigating algebraic structure of eq. (8) in wide hopping parameter ranges, we consider a uniaxial pressure applied along the a -axis, which is the stacking direction of BEDT-TTF molecules in the plane. For the pressure dependence of $t_\eta = t_\eta(P_a)$, we take extrapolation formula given by³⁰

$$t_\eta(P_a) = t_\eta(0)(1 + K_\eta P_a). \quad (9)$$

The parameters $t_\eta(0)$ and K_η are determined from the data at $P_a = 0$ given in ref. 31 and the data at $P_a = 2\text{kbar}$ given in ref. 32. The explicit values are³⁰ $t_{p1}(0) = 0.140$, $t_{p2}(0) = 0.123$, $t_{p3}(0) = -0.025$, $t_{p4}(0) = -0.062$, $t_{c1}(0) = 0.048$, $t_{c2}(0) = -0.020$, $t_{c3}(0) = -0.028$, $t_{c4}(0) = -0.028$, $K_{p1} = 0.011$, $K_{p2} = 0$, $K_{p3} = 0$, $K_{p4} = 0.032$, $K_{c1} = 0.167$, $K_{c2} = -0.025$, and $K_{c3} = K_{c4} = 0.089$.

Our purpose is to find two matrices Γ_x and Γ_y that play a role similar to σ_x and σ_y in graphene. Contrary to the Hamiltonian of graphene (1), there are other orbitals. Therefore, the situation is much more complicated. In fact, one can find Γ_x and Γ_y from numerical calculations at a given pressure P_a . However, it is hard to figure out the underlying algebraic structure. Nevertheless we show that there is a simple algebraic structure that governs the Dirac fermion spectrum of α -(BEDT-TTF)₂I₃. We assume that Γ_x and Γ_y have the following form:

$$\Gamma_x = \begin{pmatrix} 0 & 0 & e^{i\phi_x} & 0 \\ 0 & 0 & 0 & e^{i\theta_x} \\ e^{-i\phi_x} & 0 & 0 & 0 \\ 0 & e^{-i\theta_x} & 0 & 0 \end{pmatrix}, \quad \Gamma_y = \begin{pmatrix} 0 & e^{i\phi_y} & 0 & 0 \\ e^{-i\phi_y} & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{i\theta_y} \\ 0 & 0 & e^{-i\theta_y} & 0 \end{pmatrix}. \quad (10)$$

These forms are inferred from the forms of $\partial H_k / \partial k_x$ and $\partial H_k / \partial k_y$. Some components are omitted so that $\text{tr}(\Gamma_x \Gamma_y) = 0$. Furthermore, we take Γ_x and Γ_y so that $n_{kx} = \text{tr}(\Gamma_x H_k)$ depends on $t_{p1}, t_{p2}, t_{p3}, t_{p4}$ and $n_{ky} = \text{tr}(\Gamma_y H_k)$ depends on $t_{c1}, t_{c2}, t_{c3}, t_{c4}$.

If we represent a Dirac point by (k_{Dx}, k_{Dy}) , the phases in eq. (10) should depend on k_{Dx} and k_{Dy} . In order to make clear this dependence, we shift θ_x and ϕ_y as $\theta_x \rightarrow \theta_x + k_{Dx}/2$ and $\phi_y \rightarrow \phi_y - k_{Dy}/2$, respectively, and fix ϕ_x and θ_y as $\phi_x = \pi/2 + k_{Dx}/2$ and $\theta_y = \pi/2 - k_{Dy}/2$, respectively. We find that the vector field (n_{kx}, n_{ky}) has a vortex configuration in \mathbf{k} space as shown in Fig. 2 on the plane of k_x and k_y . The vortex moves in \mathbf{k} space by changing the phase parameters ϕ_y and θ_x . The chirality of Dirac fermions in α -(BEDT-TTF)₂I₃ is described by (n_{kx}, n_{ky}) by suitably choosing the phase parameters.

The phase parameters are determined by solving $(n_{k_{Dx}}, n_{k_{Dy}}) = 0$:

$$-t_{p1} \sin \frac{k_{Dx}}{2} - t_{p2} \cos \left(\theta_x - \frac{k_{Dx}}{2} \right) + t_{p3} \cos \left(\theta_x + \frac{k_{Dx}}{2} \right) - t_{p4} \sin \frac{k_{Dx}}{2} = 0, \quad (11)$$

$$t_{c1} \cos \left(\phi_y - \frac{k_{Dy}}{2} \right) + t_{c2} \cos \left(\phi_y + \frac{k_{Dy}}{2} \right) + t_{c3} \sin \frac{k_{Dy}}{2} - t_{c4} \sin \frac{k_{Dy}}{2} = 0. \quad (12)$$

The pressure dependence of the phase parameters is shown in Fig. 3. The Dirac points \mathbf{k}_D are computed by diagonalizing the Hamiltonian numerically. Figure 4 shows the pressure

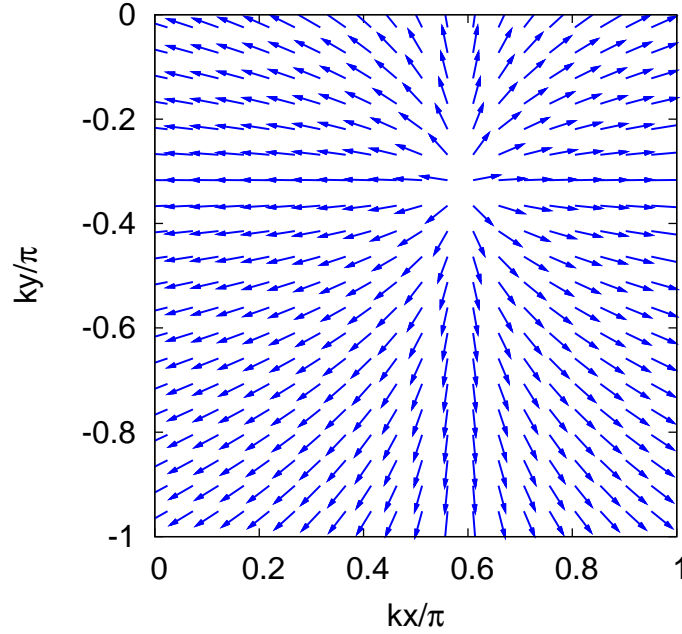


Fig. 2. The vector field (n_{k_x}, n_{k_y}) for α -(BEDT-TTF) $_2$ I $_3$ in \mathbf{k} space at $Pa = 5$ kbar. The vector field is normalized to clarify the structure around the Dirac point as in Fig. 1. The phase parameters are $\theta_x = 161.85$ degree, $\phi_y = 50.05$ degree.

dependence of the positions of the Dirac points \mathbf{k}_D . Note that the pressure dependence of θ_x is similar to that of k_{Dx} and the pressure dependence of ϕ_y is similar to that of k_{Dy} . Figure 5 shows k_{Dx} dependence of θ_x and k_{Dy} dependence of ϕ_y . We find that the phase parameters are approximately linearly dependent on the Dirac point coordinates, that is,

$$\begin{aligned}\theta_x &= \frac{2}{3} \left(k_{Dx} + \frac{3}{4}\pi \right), \\ \phi_y &= \frac{2}{3} \left(k_{Dy} + \frac{3}{4}\pi \right).\end{aligned}$$

This result demonstrates that underlying symmetry structure is rather simple despite the fact that the Hamiltonian has a complex form. The reason why we encounter the factor $2/3$ has not been clarified yet. The origin of this simple factor is left for a future study.

4. Multiorbital Hamiltonian with Dirac fermion spectrum

In the previous section, we have found matrices Γ_x and Γ_y that describe chirality of the Dirac fermions in α -(BEDT-TTF) $_2$ I $_3$. In this section, we construct a multi-orbital Dirac fermion Hamiltonian where chirality is *exactly* described by Γ_x and Γ_y . We show that the Hamiltonian has Dirac points whose positions are hopping parameter dependent and not located at symmetric points in the BZ. So characteristic features of Dirac fermions in α -(BEDT-

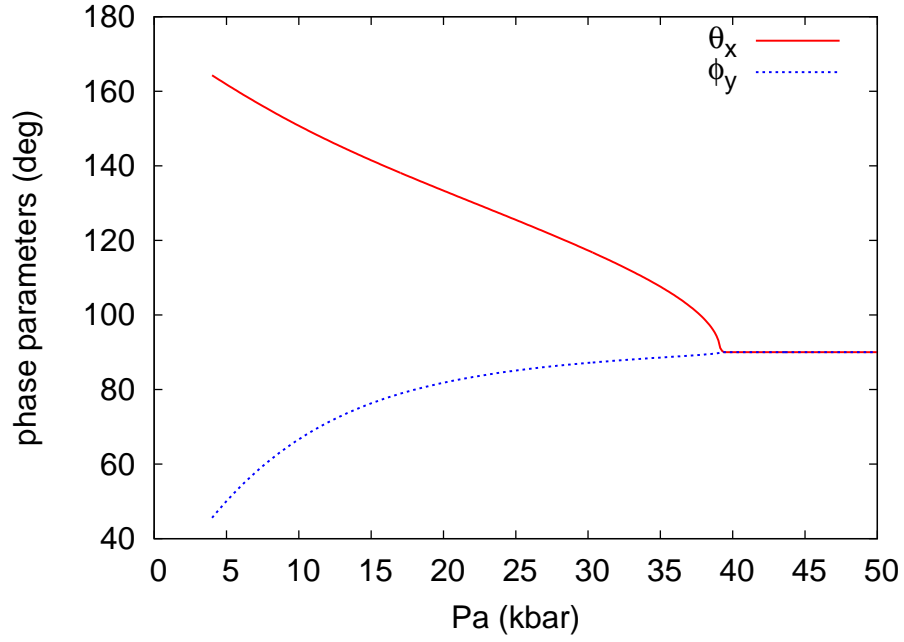


Fig. 3. Pressure dependence of the phase parameters θ_x and ϕ_y .

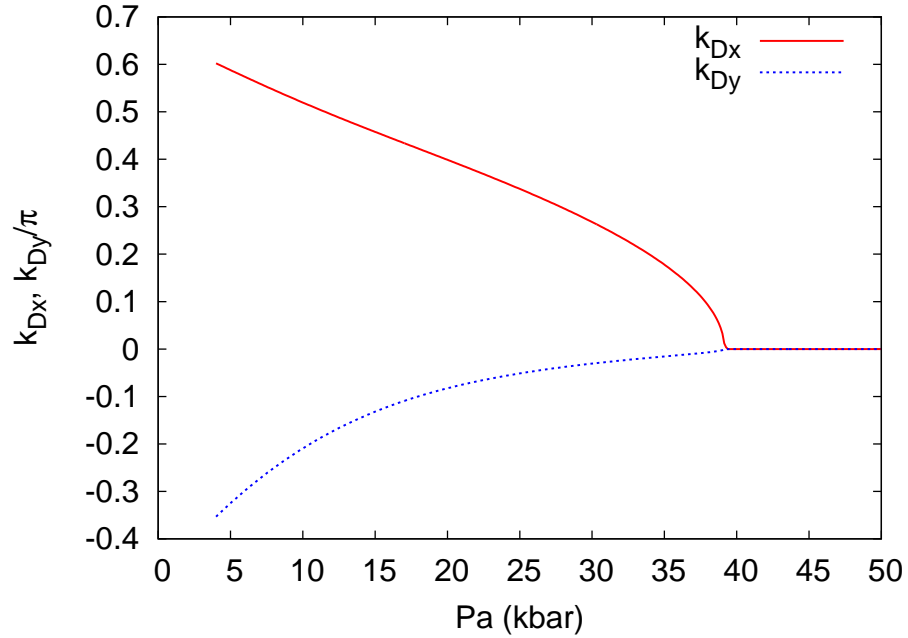


Fig. 4. Pressure dependence of the Dirac point in the third quadrant of BZ.

$\text{TTF})_2\text{I}_3$ are reproduced by this Hamiltonian.

From the form of eq. (10) and the fact that the chirality vector field is obtained by taking

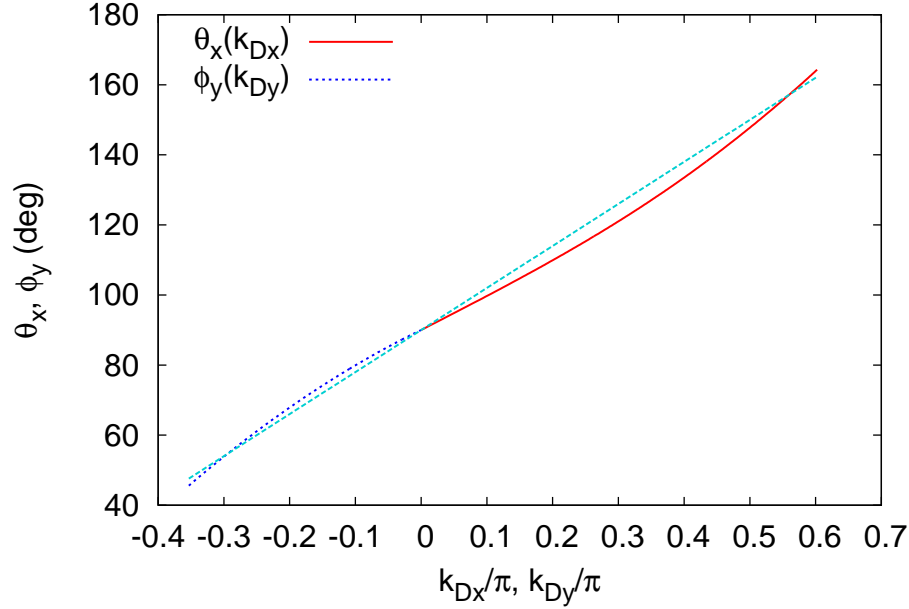


Fig. 5. The phase parameters θ_x and ϕ_y as functions of k_{Dx} and k_{Dy} , respectively. As shown by a dashed line, θ_x and ϕ_y approximately linearly depend on k_{Dx} and k_{Dy} , respectively.

trace of $\Gamma_x H_k$ and $\Gamma_y H_k$, we may consider the following Hamiltonian:

$$H_{\mathbf{k}} = \begin{pmatrix} 0 & p + qe^{-ik_y} & r + se^{ik_x} & 0 \\ p + qe^{ik_y} & 0 & 0 & t + ue^{ik_x} \\ r + se^{-ik_x} & 0 & 0 & v + we^{-ik_y} \\ 0 & t + ue^{-ik_x} & v + we^{ik_y} & 0 \end{pmatrix}. \quad (13)$$

The hopping parameters, p, q, r, s, t, u, v , and w , which are real numbers, are defined in Fig. 6 in real space. The Hamiltonian (13) is exactly diagonalized. The eigenvalues are

$$E_k^{(\pm, \pm)} = \pm \sqrt{A_k \pm \sqrt{A_k^2 - B_k^2}} \quad (14)$$

where

$$A_k = \frac{1}{2} \left(|p + qe^{-ik_y}|^2 + |r + se^{ik_x}|^2 + |t + ue^{ik_x}|^2 + |v + we^{-ik_y}|^2 \right), \quad (15)$$

$$B_k = \left| (p + qe^{-ik_y})(v + we^{ik_y}) - (r + se^{ik_x})(t + ue^{-ik_x}) \right|. \quad (16)$$

The upper two bands $E_k^{(+, +)}$ and $E_k^{(+, -)}$ touches at a point when $A_k = B_k$ is satisfied at a single \mathbf{k} point. Since there are many possibilities to satisfy this condition in general, we limit ourselves to consider a simple case where the equations $v + we^{-ik_y} = e^{i\phi} (p + qe^{-ik_y})$ and $t + ue^{ik_x} = -e^{i\phi} (r + se^{ik_x})$ are satisfied at some point (k_x, k_y) with ϕ being a constant. These

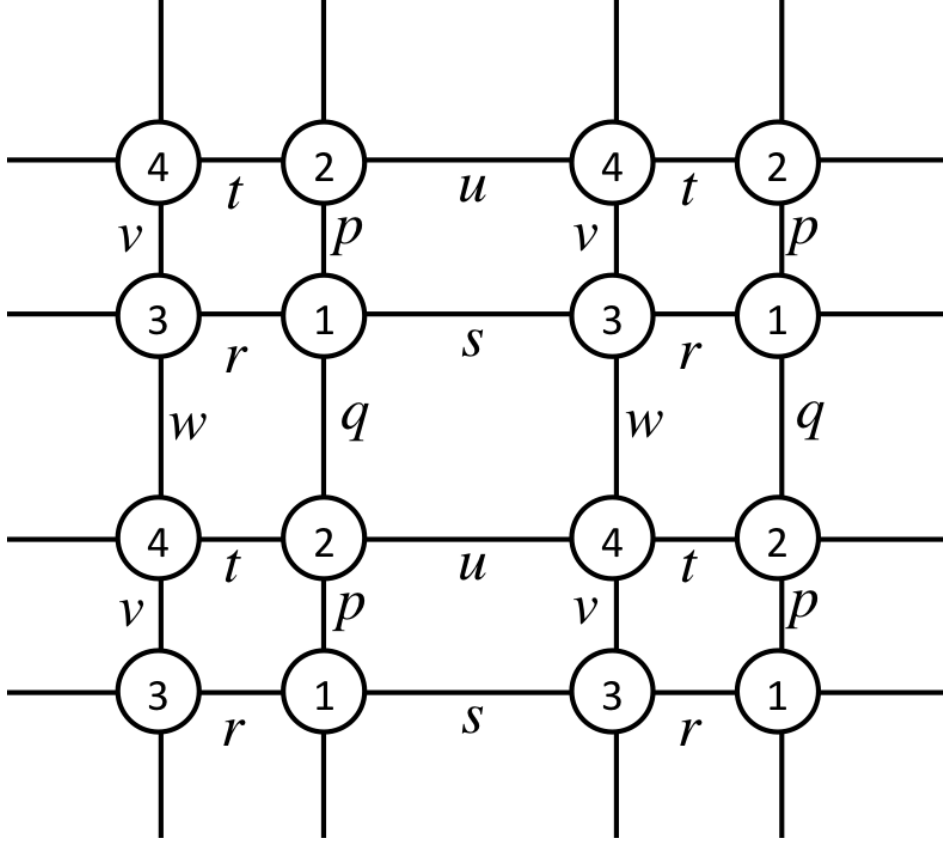


Fig. 6. The hopping parameters of the reduced Hamiltonian eq. (13). The unit cell contains four sites as in the case of α -(BEDT-TTF) $_2$ I $_3$.

equations are easily solved analytically with respect to k_x and k_y , and we find

$$k_x = \text{Im} \left[\ln \left(-\frac{t + re^{i\phi}}{u + se^{i\phi}} \right) \right],$$

$$k_y = -\text{Im} \left[\ln \left(\frac{pe^{i\phi} - v}{w - qe^{i\phi}} \right) \right].$$

with constraints $|pe^{i\phi} - v| = |w - qe^{i\phi}|$ and $|t + re^{i\phi}| = |u + se^{i\phi}|$. The constraints are solved with respect to w and s :

$$w = q \cos \phi \pm \sqrt{p^2 + v^2 - 2pv \cos \phi - q^2 \sin^2 \phi}, \quad (17)$$

$$s = u \cos \phi \pm \sqrt{r^2 + t^2 + 2rt \cos \phi - u^2 \sin^2 \phi}. \quad (18)$$

We show an example in Fig. 7 which always exhibits a zero gap state, *i.e.*, the energy of the Dirac point does not intersect either $E_k^{(+,+)}$ or $E_k^{(+,-)}$ in the BZ except at the Dirac points. We clearly see that the energy dispersion is linear around $(k_x, k_y) = (0.3587, 1.773)\pi$, which is the Dirac point. Although we do not know the analytic solution for α -(BEDT-TTF) $_2$ I $_3$ but

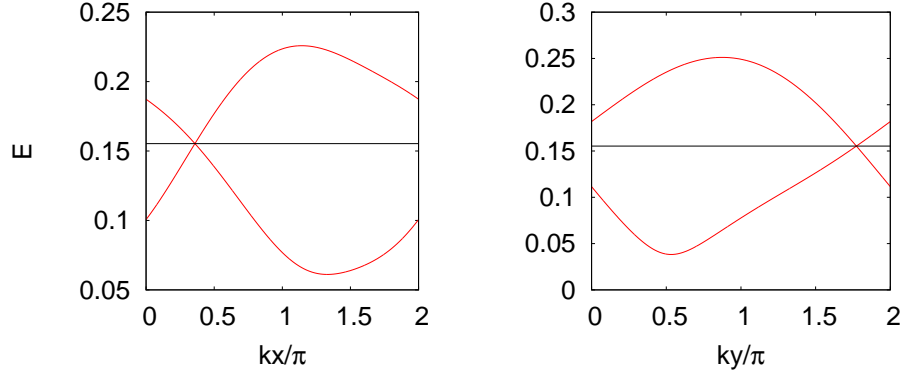


Fig. 7. The energy dispersions of the Hamiltonian (13) along k_x -axis with $k_y = 1.773\pi$ (left panel) and k_y -axis with $k_x = 0.3587\pi$ (right panel). The upper two bands, *i.e.*, $E_k^{(+,+)}$ and $E_k^{(+,-)}$ are shown. The Dirac point is at $(k_x, k_y) = (0.3587, 1.773)\pi$. The horizontal solid line is the energy of the Dirac point. The parameter values are $p = 0.08808$, $q = -0.0175$, $r = 0.1477$, $s = -0.0389$, $t = -0.025$, $u = -0.123$, $v = -0.04046$, $w = 0.1015$, and $\phi = 70$ degree. We set these values using the hopping parameter values of α -(BEDT-TTF) $_2$ I $_3$ at $P_a = 5$ kbar except for s and w . The parameters s and w are determined from eqs. (17) and (18).

we believe that the Hamiltonian (13) captures essential symmetric properties of the Dirac fermions of α -(BEDT-TTF) $_2$ I $_3$.

The fact that the Dirac point moves in the BZ by changing the hopping parameters is demonstrated in Fig. 8. Therefore, the Hamiltonian eq. (13) shares the feature of the moving Dirac points in the BZ with α -(BEDT-TTF) $_2$ I $_3$. We show one Dirac point $\mathbf{k}_D = (k_{Dx}, k_{Dy})$ in Fig. 8. The other Dirac point is at $(-k_{Dx}, -k_{Dy})$ by symmetry.

It is interesting to point out a possible relationship between the model and the π -flux state that was originally proposed for the two-dimensional antiferromagnetic Heisenberg model.³³ We shall discuss that α -(BEDT-TTF) $_2$ I $_3$ is characterized by a π -flux state in a multi-orbital system in a future publication.

5. Summary

To summarize, we have investigated underlying algebraic structure of the Dirac fermion spectrum of α -(BEDT-TTF) $_2$ I $_3$. We have found that chirality of Dirac fermions in α -(BEDT-TTF) $_2$ I $_3$ is well described by the matrices Γ_x and Γ_y defined by eq. (10). The phase factors in Γ_x and Γ_y have intimate relationships with the position of the Dirac point in the BZ, and we have found a simple relationship between them. A reduced form of the Hamiltonian has been constructed from Γ_x and Γ_y . The Dirac point of the reduced Hamiltonian moves in the BZ by changing hopping parameters. Although the analytic expression for the Dirac points of α -(BEDT-TTF) $_2$ I $_3$ is still unknown, our reduced Hamiltonian has the analytic expression for the

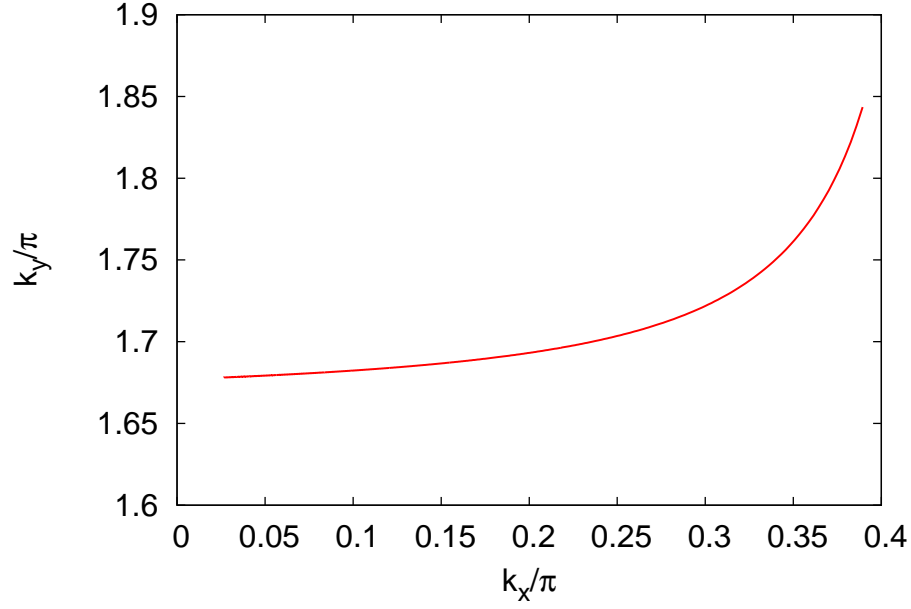


Fig. 8. The motion of the Dirac point in the BZ. We take the hopping parameters as described in Fig. 7 with changing P_a .

Dirac points. Therefore, the reduced Hamiltonian is a useful model to unveil the mechanism of stabilizing the Dirac fermion spectrum in α -(BEDT-TTF)₂I₃.

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